

(19) World Intellectual Property
Organization
International Bureau



(43) International Publication Date
6 May 2005 (06.05.2005)

PCT

(10) International Publication Number
WO 2005/040985 A2

- (51) International Patent Classification⁷: **G06F**
- (21) International Application Number:
PCT/US2004/034618
- (22) International Filing Date: 20 October 2004 (20.10.2004)
- (25) Filing Language: English
- (26) Publication Language: English
- (30) Priority Data:
10/689,313 20 October 2003 (20.10.2003) US
- (71) Applicant (for all designated States except US): **CERNO BIOSCIENCE LLC** [US/US]; Suite 13, 5 Science Park, New Haven, Connecticut 06511 (US).
- (72) Inventors; and
- (75) Inventors/Applicants (for US only): **WANG, Yongdong**

[US/US]; 73 Moriarity Drive, Wilton, Connecticut 06897 (US). **GU, Ming** [US/US]; 416 Schindler Drive, Yardley, Pennsylvania 19067 (US).

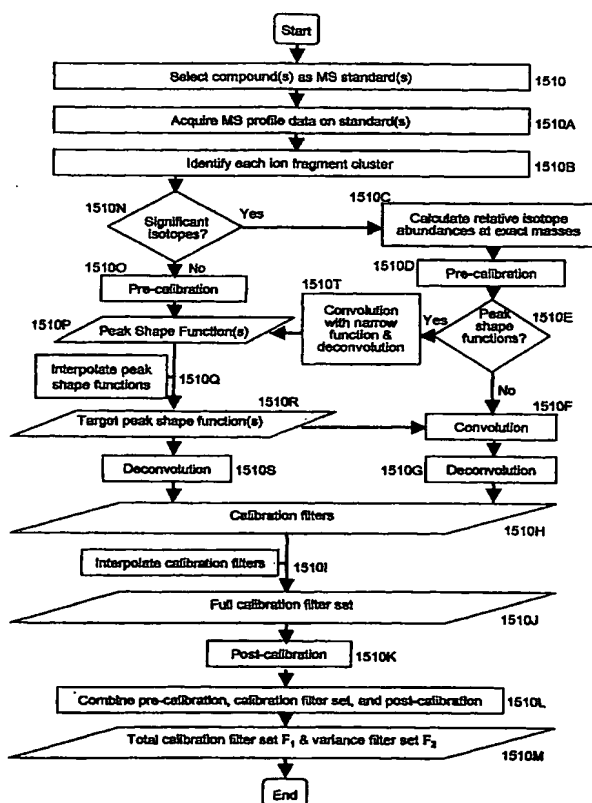
(74) Agent: **AKER, David**; Attorney at Law, 23 Southern Road, Hartsdale, New York 10530 (US).

(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM,

[Continued on next page]

(54) Title: METHODS FOR CALIBRATING MASS SPECTROMETRY (MS) AND OTHER INSTRUMENT SYSTEMS AND FOR PROCESSING MS AND OTHER DATA



(57) Abstract: A method for obtaining at least one calibration filter for a Mass Spectrometry (MS) instrument system. Measured isotope peak cluster data in a mass spectral range is obtained for a given calibration standard. Relative isotope abundances and actual mass locations of isotopes corresponding thereto are calculated for the given calibration standard. Mass spectral target peak shape functions centered within respective mass spectral ranges are specified. Convolution operations are performed between the calculated relative isotope abundances and the mass spectral target peak shape functions to form calculated isotope peak cluster data. A deconvolution operation is performed between the measured isotope peak cluster data and the calculated isotope peak cluster data after the convolution operations to obtain the at least one calibration filter. Provisions are made for normalizing peak widths, combining internal and external calibration, and using selected measured peaks as standards. Aspects of the methods are applied to other analytical instruments.

WO 2005/040985 A2



ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

Published:

- *without international search report and to be republished upon receipt of that report*